ITR: Development of Quantitative Coarse-grained Models for Simulation of Polyolefin Blends

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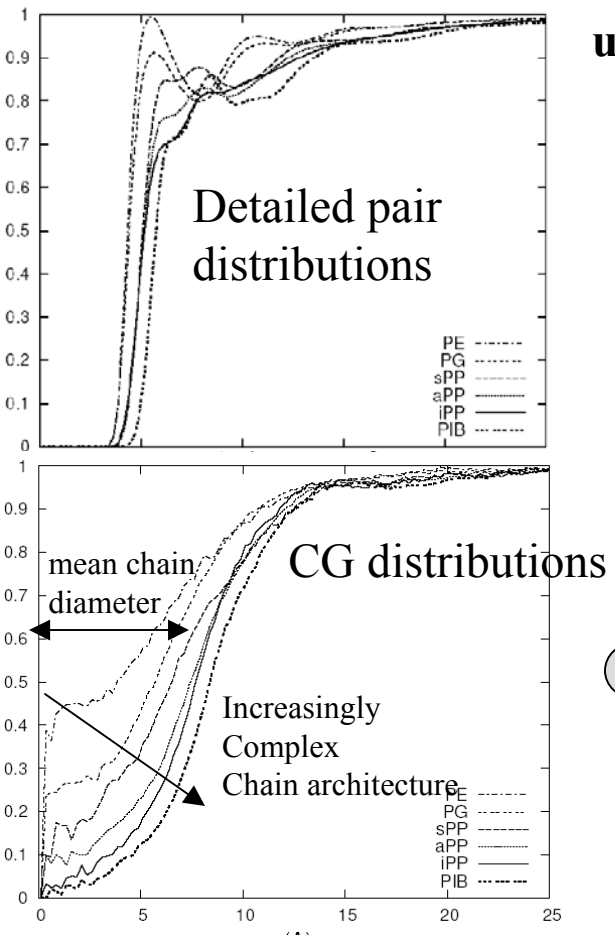
Atomistic simulation of long chain polymers are computationally daunting. Over the first year of the ITR we developed a coarse-graining method that reduces the computation effort without the loss of chemical information. We have applied this method to simulate long chain polyethylene and tested it through predictions of radius of gyration, structure etc.

Recently, we have extended this method to other poly-olefins that differ subtly in their molecular architecture – syndiotactic, atactic, and isotactic polypropylene, and polyisobutylene. Two important lengthscales can be quantified through these calculations – the chain persistence length and the mean chain diameter. Detailed simulations obscure the latter quantity due to numerous peaks from local polymer structure, and has been deduced, to date from macroscopic properties and persistence length. Coarse-graining process integrates over these details without the loss of chemical detail allowing quantification of the second lengthscale. This information will be used in the near future to understand entanglements in polymers.



Central idea underlying theCG method

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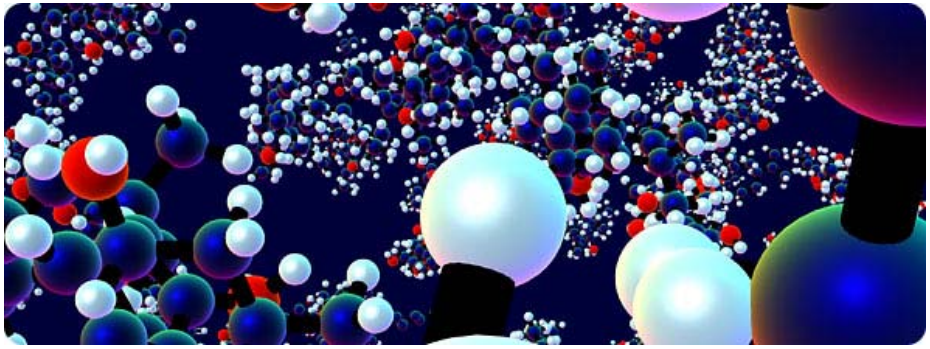
Education and Outreach

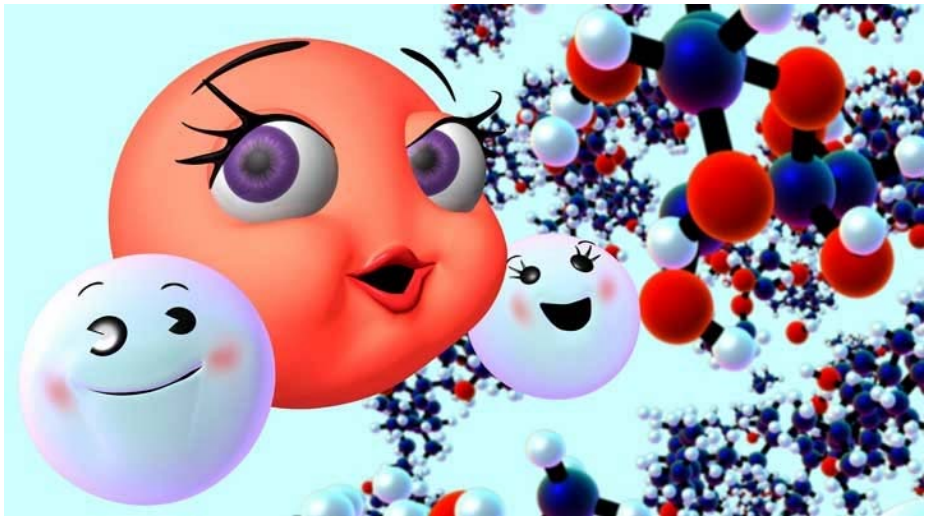
• **The New Visions Project**: We are actively participating in the Questar's New Visions project. The goal is to expose high school students to career paths in math, engineering, technology, and science. We present lectures and lab demonstrations each selmester and have received enthusiastic response.

• **The Molecularium:** Primarily funded by the NSEC (DMR) at Rensselaer, the idea is to make entertaining animation movies about the molecular world using simulation data and basic molecular concepts. As shown, simulations performed under ITR have been successfully ported to animation software. The first 20 minute Molecular show will be available in the local planetarium for viewing in early 2005.

• **Course development**: Profs. Kumar and Schadler developed a Nanotechnology course for undergraduate and graduate students. The course was well received and will be offered again.



Rendering of a polyethylene molecule



A water molecule with characters: oxy, hydra, and hydro, admiring a polymer chain